UMP-98/?

The Lanczos Algorithm for extensive Many-Body Systems in the Thermodynamic Limit

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February 7, 2008

Abstract

We establish rigourously the scaling properties of the Lanczos process applied to an arbitrary extensive Many-Body System which is carried to convergence $n \to \infty$ and the thermodynamic limit $N \to \infty$ taken. In this limit the solution for the limiting Lanczos coefficients are found exactly and generally through two equivalent sets of equations, given initial knowledge of the exact cumulant generating function. The measure and the Orthogonal Polynomial System associated with the Lanczos process in this regime are also given explicitly. Some important representations of these Lanczos functions are given, including Taylor series expansions, and theorems controlling their general properties are proven.

PACS: 05.30.-d, 11.15.Tk, 71.10.Pm, 75.10.Jm

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I. Introduction

The Lanczos Algorithm is one of the few reliable and general methods for computing the ground state and excited state properties of strongly interacting quantum Many-body Systems. It has been traditionally employed as a numerical technique on small finite systems, with attendant round-off error problems, although the main obstacle to its further development has been the rapid growth of the number of basis states with system size. The reader is referred to a review of the applications of this method[1] in strongly correlated electron problems. In this work we examine the Lanczos process in the context of the extensive quantum Many-Body Systems, where it is employed entirely in an exact manner and where the thermodynamic limit is taken. So in complete contrast to the traditional use of the Lanczos algorithm - we completely circumvent the issues of loss of orthogonality due to round-off errors and the inability to approach the thermodynamic limit because of the requirement to construct a full basis on the cluster. The systems we have in mind are those with an infinite number of degrees of freedom, yet are extensive, in that all total averages of any physical quantity scale linearly with the numbers of degrees of freedom however quantified. These would include all condensed matter systems with sufficiently local interactions (the precise conditions need to be clarified, but it is clear which specific systems obey extensivity) and Quantum Field Theories, with the proviso that the spectrum is bounded below (in some cases there is also an upper bound too).

After noting some of the advantageous features of the algorithm in general we discuss the scaling behaviour of the Lanczos Process as it approaches convergence and as the thermodynamic limit is taken. Central to this approach is the manifestation of extensivity through a description based on the Cumulant Generating Function, which we take to be given. We then derive a set of general integral equations which define the scaled Lanczos functions in the thermodynamic limit, which can be explicitly and exactly solved for certain integrable models, or employed in a truncated manner for non-integrable models. An alternative formulation is also given which expresses the equivalence of the Lanczos Process with the continuum Toda Lattice Model treated as a boundary value problem. Finally we state some general results concerning the behaviour of the Lanczos functions.

II. The Lanczos Process, Orthogonal Polynomials and Moments

The Lanczos Algorithm or Process[2, 3, 4] begins with a trial state $|\psi_0\rangle$ appropriate to the model and the symmetries of the phase being investigated. From this the Lanczos recurrence generates a sequence of orthonormal states $\{|\psi_n\rangle\}_{n=1}^{\infty}$ and Lanczos coefficients $\{\alpha_n(N)\}_{n=0}^{\infty}$ and $\{\beta_n(N)\}_{n=1}^{\infty}$, thus

$$\hat{H}|\psi_n\rangle = \beta_n|\psi_{n-1}\rangle + \alpha_n|\psi_n\rangle + \beta_{n+1}|\psi_{n+1}\rangle \ , \tag{1}$$

with the Lanczos coefficients being defined

$$\begin{aligned} \alpha_n &= \langle\psi_n|\hat{H}|\psi_n\rangle \ , \\ \beta_n &= \langle\psi_{n-1}|\hat{H}|\psi_n\rangle \ . \end{aligned} \tag{2}$$

We distinguish a total or extensive operator or variable such as H from its density or intensive counterpart by $\hat{H}$. In this basis the transformed Hamiltonian takes the following tridiagonal form

$$T_n = \begin{pmatrix} \alpha_0 & \beta_1 & & & & \\ \beta_1 & \alpha_1 & \beta_2 & & & \\ & & \ddots & & & \\ & & & \beta_{n-1} & \alpha_{n-1} & \beta_n \\ & & & & \beta_n & \alpha_n \end{pmatrix} \ . \tag{3}$$

As such the Lanczos process is one of the Krylov subspace methods[5], in that at a finite step n, the eigenvectors belong to the Krylov Subspace Span$\{|\psi_0\rangle, \hat{H}|\psi_0\rangle, \hat{H}^2|\psi_0\rangle, \ldots \hat{H}^n|\psi_0\rangle\}$.

In the Many-Body context one would iterate the Lanczos Process until termination whereupon the Hilbert space is exhausted (at this point one of the $\beta_{n_T} = 0$, where n_T is the dimension of the Hilbert space in the sector defined by the ground state), or until the process has converged according to some arbitrary criteria $n \to n_C$. Then one would perform the thermodynamic limit $N \to \infty$ where it should be understood that the above conclusion of the Lanczos process is also dependent on the system size, that is to say $n_T(N), n_C(N)$. These cutoffs are monotonically increasing functions of the system size so they will all tend to ∞ in the thermodynamic limit as well. Taking the limits in the reverse order clearly leads to nonsensical results, as taking $N \to \infty$ with n fixed produces $\alpha_n \to c_1$ and $\beta_n \to 0$. The great virtue of the Lanczos process is that it can be shown to converge essentially exponentially fast with respect to iteration number, using the Kaniel-Paige-Saad exact bounds[6, 7, 8] for the rate of convergence. This means that convergence occurs within a very small subspace of the total Hilbert space, so that $n_C << n_T$.

The Lanczos process is entirely equivalent to the 3-term recurrence for an Orthogonal Polynomial System[9, 10, 11], however we consider a slight generalisation of the preceding process to one with a single parameter evolution (a "time" t). In this construction we are continuing a development begun by Lindsay[12] and Chen and Ismail[13], which will lead to some powerful tools in treating the Lanczos process. The measure, or that component which is absolutely continuous, is defined by the weight function

$$w(\epsilon, t) = e^{-u(\epsilon)+tN\epsilon} \ , \tag{4}$$

on the real line $\epsilon \in \mathbb{R}$. Our system under study is described by the initial value of the system at $t = 0$ and often we will suppress this argument for the sake of simplicity. This measure defines

a system of monic Orthogonal Polynomials $\{P_n(\epsilon,t)\}_{n=0}^{\infty}$ with an orthogonality relation

$$\int_{-\infty}^{+\infty} d\epsilon \; w(\epsilon,t) P_m(\epsilon,t) P_n(\epsilon,t) = h_n(t)\delta_{mn} \; , \tag{5}$$

and normalisation $h_n(t)$. This is equivalent to the following three-term recurrence relation

$$P_{n+1}(\epsilon,t) = (\epsilon - \alpha_n(t))P_n(\epsilon,t) - \beta_n^2(t)P_{n-1}(\epsilon,t) \; , \tag{6}$$

with the recursion coefficients $\alpha_n(t)$ real for $n \geq 0$ and $\beta_n^2(t)$ real and positive for $n > 0$. By convention we take $\beta_0^2 = 1$. It can be readily shown that the Lanczos coefficients are given in terms of the normalisation thus

$$\begin{aligned} \alpha_n(t) &= \frac{1}{N h_n(t)} \frac{d}{dt} h_n(t) \; , \\ \beta_n^2(t) &= \frac{h_n(t)}{h_{n-1}(t)} \; . \end{aligned} \tag{7}$$

The direct connection between the Lanczos Process and the OPS are given by the determinant relation of the characteristic polynomial

$$P_{n+1}(\epsilon) = (-)^{n+1} |T_n - \epsilon I_{n+1}| \; , \tag{8}$$

so that the zeros of the Orthogonal Polynomial are eigenvalues of Hamiltonian.

Some comments are in order regarding the differences, or more accurately the special character, of these Orthogonal Polynomials with respect to the generic OPS or with some of the scaling versions of OPS[14]. These OPS have been termed Many-Body OPS, but could be equally described as extensive OPS. They all have an additional, essential parameter to the generic OPS, the system size N, which appears in both the gross scaling factors (the 'external' scaling such as in the energy densities ϵ defined by $E = N\epsilon$), but also internally in the 3-term recurrence coefficients, in the Polynomials themselves and in other derived quantities. The internal dependence in the Lanczos coefficients on the system size is not at all apparent and the most transparent way that extensive scaling properties can be exhibited is through the Cumulant Generating Function, (CGF), which hitherto has played no role in Orthogonal Polynomial Theory. In fact the CGF is central to this class of OPS rather than the moments, and is in a practical sense the starting point in any application of the Formalism to physical Models. For all models it is clear that the ground state energy E_0 is proportional to N and unbounded in the thermodynamic limit, and similarly the total Lanczos coefficients (as opposed to the densities) are unbounded as $n \to \infty$ for fixed N. When everything is recast in terms of densities the spectrum is bounded below by ϵ_0 and in many models will also be bounded above, and similarly the density Lanczos coefficients are bounded. Another difference that Many-Body OPS exhibit in comparison to general OPS is, as we have noted above, the three-term recurrence will terminate exactly at $n = n_T$, although this will never present any problems as this is exponentially large.

The Lanczos process is intimately connected with the Hamburger moment problem[15, 16], via the Resolvent operator

$$R(\epsilon) = \langle \frac{1}{\epsilon - \hat{H}} \rangle \qquad \epsilon \notin \mathrm{Supp}[d\rho] \; . \tag{9}$$

Its formal Laurent series establishes a direct link with Hamiltonian moments

$$R(\epsilon) = \sum_{i=0}^{\infty} \frac{\mu_i}{\epsilon^{i+1}} \; , \tag{10}$$

where these moments are defined as expectation values with respect to the trial state referred to above

$$\mu_n \equiv \langle \hat{H}^n \rangle \ , \qquad \mu_0 = 1 \ . \tag{11}$$

The resolvent has a real Jacobi-fraction continued fraction representation[17, 18]

$$R(\epsilon) = -\mathbf{K}_{n=0}^{\infty} - \left(\frac{\beta_n^2}{\epsilon - \alpha_n} \right) \ , \tag{12}$$

with elements coming from the Lanczos coefficients.

An equivalent description to that of the Hamiltonian moments is to formulate everything in terms of cumulants or connected moments[19, 20] $\{\nu_n\}_{n=1}^{\infty}$, and to ignore all corrections which vanish in the thermodynamic limit $N \to \infty$. Cumulants scale directly with the size of the system so that for the extensive Many-Body Problem we have

$$\nu_n = c_n N + \mathrm{o}(1) \tag{13}$$

in the ground state sector, or

$$\nu_n = c_n N + m_n + \mathrm{o}(1) \tag{14}$$

in any other sector[21]. This also means that no finite-size scaling can be performed given that only the limiting quantities are retained here and boundary condition effects do not appear. The foundation ingredient is the Moment Generating Function which is related to the Cumulant Generating Function in the following way.

Definition 1 *The Moment Generating Function (MGF) $M(t)$ and the Cumulant Generating Functions (CGF) $F(t)$ are defined by,*

$$M(t) \equiv \langle e^{tH} \rangle = \sum_{n=0}^{\infty} \mu_n \frac{t^n}{n!} = \exp\left(\sum_{n=1}^{\infty} \nu_n \frac{t^n}{n!} \right) \equiv \exp(NF(t)) \ . \tag{15}$$

Some examples of Cumulant Generating Functions include the isotropic XY model using the z-polarised Néel state as the trial state[22]

$$F(t) = \frac{1}{\pi} \int_0^{\pi/2} dq \log\cosh(t\cos q) \ , \tag{16}$$

and the Ising model in a transverse field using the disordered state as the trial state, and coupling constant x[23]

$$F(t) = \frac{1}{2\pi} \int_0^{\pi} dq \ \ln\left[\cosh(2t\epsilon_q) - \frac{(\cos q + x)}{\epsilon_q} \sinh(2t\epsilon_q) \right] \ , \tag{17}$$

where the quasiparticle energies ϵ_k are defined by $\epsilon_q^2 = 1 + x^2 + 2x\cos q$.

Definition 2 *The Determinants of the Moment Matrices $\Delta_n(t)$ for $n \geq 0$ are defined by the Hankel form -*

$$\Delta_n(t) = |M^{(i+j-2)}(t)|_{i,j=1}^{n+1} \ . \tag{18}$$

The direct relationship from moments to the Lanczos coefficients which is established in this way is via the construction of a sequence of Hankel determinants of the Moment Matrices and their Selberg-type integral representation[9]

$$\Delta_n(t) = \frac{1}{(n+1)!} \int_{-\infty}^{+\infty} \prod_{k=1}^{n+1} d\epsilon_k \; w(\epsilon_k, t) \prod_{1 \le i < j \le n+1} |\epsilon_i - \epsilon_j|^2 \; . \tag{19}$$

These determinants are related to the normalisations via

$$\Delta_n(t) = \prod_{j \le n} h_j(t) \; . \tag{20}$$

Definition 3 *Our final definition, that of the Lanczos L-function, is*

$$N^2 L_n(t) = \frac{\Delta_n(t)\Delta_{n-2}(t)}{\Delta^2_{n-1}(t)} \; , \tag{21}$$

for $n \ge 1$ and $L_0(t) = M(t)$.

The converse result is then

$$\Delta_n(t) = N^{n(n+1)} \prod_{k=0}^{n} L_k^{n+1-k}(t) \; , \tag{22}$$

for $n \ge 1$. From these the Lanczos coefficients are given simply by

$$\begin{aligned} \alpha_n(t) &= \frac{1}{N} \sum_{j=0}^{n} \frac{L'_j(t)}{L_j(t)} \; , \\ \beta^2_n(t) &= L_n(t) \; . \end{aligned} \tag{23}$$

Theorem 1 *The equation of motion for the Lanczos L-functions is*

$$L_n(t) = \frac{1}{N} \sum_{j=1}^{n} \frac{j}{N} D_t^2 \log L_{n-j}(t) \; . \tag{24}$$

with the initial condition on the recurrence given by $\log L_0(t) = NF(t)$ *for all* t.

The advantage of introducing evolution into the Lanczos Process is that Sylvester's Theorem applied to the Hankel determinants[24],

$$\Delta_{n+1}(t)\Delta_{n-1}(t) = \Delta_n(t)\Delta''_n(t) - \left(\Delta'_n(t)\right)^2 \tag{25}$$

so that the theorem follows directly from this.□

The first few members of the Lanczos L-sequence are

$$\begin{aligned} L_1(t) &= \frac{1}{N} F''(t) \; , \\ L_2(t) &= \frac{2}{N} F''(t) + \frac{1}{N^2} \frac{F^{(2)}F^{(4)} - (F^{(3)})^2}{(F^{(2)})^2} \; . \end{aligned} \tag{26}$$

The consequence of Sylvester's theorem for the evolution of the Δ_n is the following theorem

Theorem 2 *The* $\Delta_n(t)$ *obey the following differential-difference equation*

$$\exp\{\log\Delta_{n+1} + \log\Delta_{n-1} - 2\log\Delta_n\} = D_t^2 \log\Delta_n \ , \tag{27}$$

with the boundary value $\log\Delta_0 = NF(t)$ *and conventionally* $\Delta_{-1} = 1$.

This follows directly from Sylvester's Identity.□

This evolution equation is just the finite Toda Lattice equation of motion[25], and this point has been previously noted in Ref. [13].

III. Scaling in the Thermodynamic Limit

As was discussed earlier there are two limiting processes that one must consider when the thermodynamic limit is taken in the Lanczos Algorithm, both $n, N \to \infty$, and the issue then is what mutual relationship exists between them in the limit. One can view this limiting process in the $1/n$ vs. $1/N$ plane and then consider along what types of paths must one approach the origin. We shall find that the general relationship is $n, N \to \infty$ with $s \equiv n/N$ fixed, although for systems at criticality it seems inevitable that s will become unbounded in the analysis. A consequence of these ideas is the confluence property of the Lanczos coefficients as $n, N \to \infty$ at fixed $s = n/N$

$$\begin{aligned} \alpha_n(N) &= \alpha(s) + \mathrm{O}(1/N) \ , \\ \beta_n^2(N) &= \beta^2(s) + \mathrm{O}(1/N) \ . \end{aligned} \tag{28}$$

There are a number of ways to see this approach to the thermodynamic limit.

Using the explicit forms connecting cumulants and moments, and a direct evaluation of the Hankel determinants one can prove[26] for general n and N that the Lanczos coefficients have a leading order scaling in $s = n/N$ for the first two orders of an expansion in large N. Actually this expansion is valid for all n not just for large values and thus includes all the subdominant contributions. Thus

$$\begin{aligned} \alpha_n =& c_1 N + n \left[\frac{c_3}{c_2} \right] \\ & + \frac{1}{2} n(n-1) \left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{2c_2^4} \right] \frac{1}{N} \\ & + \dots \ , \end{aligned} \tag{29}$$

for $n \geq 0$, and

$$\begin{aligned} \beta_n^2 = & n c_2 N + \frac{1}{2} n(n-1) \left[\frac{c_2c_4 - c_3^2}{c_2^2} \right] \\ & + \frac{1}{6} n(n-1)(n-2) \left[\frac{-12c_3^4 + 21c_2c_3^2c_4 - 4c_2^2c_4^2 - 6c_2^2c_3c_5 + c_2^3c_6}{2c_2^5} \right] \frac{1}{N} \\ & + \dots \ , \end{aligned} \tag{30}$$

for $n \geq 1$. However this approach cannot be generalised to higher orders and therefore for the full exact Lanczos coefficients. The first two terms in the above expansions were also proven by Lindsay using the Sylvester Identity in the statistical context[12] but no further, while this form for the higher terms (but finite numbers) was conjectured in Reference[27]. We shall find that use of the Sylvester Identity allows one to very easily recover this result, to in fact go to much higher orders in constructing explicit forms and to prove this type of scaling in a completely general way.

Lemma 1 *The Lanczos L-function $L_n(t, N)$ is a rational function of $1/N$ for fixed n, and all t.*

The Difference-Differential Eq. (24) is of finite order in j/N and t, so the result follows.□

Also for fixed n we have

$$\lim_{N \to \infty} L_n(t, N) = 0 \ , \tag{31}$$

and specifically the leading order term is $\mathrm{O}(N^{-1})$ which arises from the $j=n$ term in the sum. Therefore we can expand this function in a descending series in N^{-1}, thus

$$L_n(t,N) = \sum_{p\geq 1} \frac{l_{np}(t)}{N^p} \ , \tag{32}$$

and defining the connected series related by

$$\sum_{p\geq 1} \frac{m_{np}(t)}{N^p} \equiv \log\left(1+\sum_{p\geq 1}\frac{l_{np+1}/l_{n1}}{N^p}\right) \ . \tag{33}$$

This last relation can be rendered into an explicit form

$$m_{np} = -\sum_{\sum_i q_i r_i = p} (\sum_i q_i - 1)! \prod_i \frac{1}{q_i!}\left(\frac{-l_{nr_i+1}}{l_{n1}}\right)^{q_i} \ . \tag{34}$$

It is actually necessary to perform an expansion of this type because it combines the iteration number (n) dependence of the numerator and denominator which are both essential in the following results.

Then one can establish a hierarchy of equations for these coefficients

$$\begin{aligned} l_{n1}(t) &= nF''(t) \ , \\ l_{n2}(t) &= \sum_{j=1}^{n-1} jD_t^2 \log l_{n-j1}(t) \ , \\ l_{np}(t) &= \sum_{j=1}^{n-1} jm''_{n-jp-2}(t) \qquad \text{for } p\geq 3 \ , \end{aligned} \tag{35}$$

for $n\geq 1$ whilst for $n=0$ we have $l_{np}(t)=0$ as $L_0(t,N)=\exp(NF(t))$. The first members of this hierarchy can be easily solved for yielding

$$\begin{aligned} l_{n1}(t) &= nF''(t) \ , \\ l_{n2}(t) &= \frac{1}{2}n(n-1)\frac{F^{(2)}F^{(4)}-(F^{(3)})^2}{(F^{(2)})^2} \ , \\ l_{n3}(t) &= \frac{1}{12}n(n-1)(n-2)\left(\frac{F^{(2)}F^{(4)}-(F^{(3)})^2}{(F^{(2)})^3}\right)^{(2)} \ , \end{aligned} \tag{36}$$

and from these it is easy to establish the leading order terms already found in Eq. (29,30).

Lemma 2 *The hierarchy coefficients $l_{np}(t), m_{np}(t)$ are polynomials in n.*

These coefficients are constructed from a finite difference equation in n. □

Theorem 3 *The hierarchy coefficients $l_{np}(t), m_{np}(t)$ are polynomials of degree p in n.*

This is proved by induction on p using the hierarchy equations. If we take $l_{jq}(t)$ to be of degree $q\leq p-2$ in n then similarly for $m_{jq}(t)$ and $m''_{jq}(t)$. Now for any polynomial $P(n)$ of degree $p-2$ in its argument then

$$\sum_{j=1}^{n-1} jP(n-j) \ , \tag{37}$$

is a pth degree polynomial. Thus the recurrence, Eq. (35), establishes that l_{n+1p} is also a pth degree polynomial.□

From this result it is clear that the limiting forms of the Lanczos coefficients $\alpha_n(N), \beta_n^2(N)$ exist when $n, N \to \infty$ with n/N fixed. If the ratio is not kept constant in this limiting operation, say with $n = \mathrm{o}(N)$ then the Lanczos coefficients will vanish in the limit, while if the reverse is true $N = \mathrm{o}(n)$ then there will be divergent terms in the limit.

Given that the scaling Lanczos coefficients have been established then all the exact theorems for the ground state properties[28, 29] that were predicated on this result now are established. The first example of these theorems was the one for the ground state Energy Density,

$$\epsilon_0 = \inf_{s \in \mathbb{R}^+} [\alpha(s) - 2\beta(s)] \ , \tag{38}$$

which also has an analogue for the top of the spectrum, if this exists

$$\epsilon_\infty = \sup_{s \in \mathbb{R}^+} [\alpha(s) + 2\beta(s)] \ . \tag{39}$$

For many models these Lanczos Functions will be bounded on the positive real axis, and have limits as $s \to \infty$ on the real line. So there is a superficial similarity to classes of Orthogonal Polynomials whose 3-term recurrence coefficients have limiting values, such as the S-class, the M-class, or the $M(a, b)$ classes[14].

IV. The extensive Measure

It is necessary to determine the OPS measure, its weight function $w(\epsilon)$, and this is not generally known at the outset, but rather the Cumulant Generating Function is. In fact it seems to be the case that the measures are not exactly expressible in simple terms, but the CGF or characteristic functions are. There is of course a direct route from a model system and a trial state to the Lanczos coefficients, but from many points of view including practical considerations the route beginning with a cumulant description is more useful.

Theorem 4 *Given that the cumulant generating function $F(-t)$ is analytic for $\Re(t) > 0$ and in the neighbourhood of the origin $t = 0$ the OPS weight function $w(\epsilon)$ has the following asymptotic development in the thermodynamic limit $N \to \infty$,*

$$w(\epsilon) = \sqrt{\frac{N}{2\pi F^{(2)}(\xi)}} e^{N[-\epsilon\xi + F(\xi)]} + \mathrm{O}(N^{-1/2}) \ , \tag{40}$$

where the function $\xi(\epsilon)$ is defined implicitly by

$$\epsilon = F'(\xi) \ . \tag{41}$$

Starting with the definition of the cumulant generating function $F(t)$

$$\langle e^{tH} \rangle \equiv \exp\{NF(t)\} = \exp\left\{ N \sum_{n=1}^{\infty} \frac{c_n}{n!} t^n \right\} \ . \tag{42}$$

We assume here that this infinite series is not just formal but actually exists, that is it has a finite radius of convergence in addition to its analytic character for $\Re(t) < 0$. However the Moment Generating Function is simply the analytic continuation of the characteristic function and this continuation is possible given its analyticity, so that a Fourier inversion of this will yield the weight function,

$$\begin{aligned} w(\epsilon) &= \frac{N}{2\pi} \int_{i\gamma-\infty}^{i\gamma+\infty} dt\ e^{N[-it\epsilon + F(it)]} \ , \\ &= \frac{N}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} dt\ e^{N[t\epsilon + F(-t)]} \qquad \Re(\gamma) > 0 \quad . \end{aligned} \tag{43}$$

One does not require the exact inversion but only the leading order in N in a steepest descent approximation. In an asymptotic analysis the relevant function is

$$g(t) = t\epsilon + F(-t) \ , \tag{44}$$

which is analytic for all $\Re(t) > 0$. We will assume the existence of a stationary point which occurs at t_0

$$\epsilon = F'(-t_0) \ , \tag{45}$$

and is assumed to be unique. This point is evidently real because the energy density is real and the CGF is a real function of a real argument (here we define $\xi = -t_0$ for convenience). One requires the inversion of this relation for $\xi(\epsilon)$ and this is guaranteed by the Implicit Function Theorem because $F^{(2)}(\xi) > 0$. This latter condition also implies that the saddle point is of order unity. Indeed one clearly has the case of $F^{(2)}(t) > 0$ for real values of t in the neighbourhood of the saddle point and $F^{(2)}(t) < 0$ for imaginary values of t in the same

neighbourhood. Thus the path of steepest descent through the saddle point is parallel to the imaginary axis. One can then apply the standard saddle point analysis, see Wong[30] Section II.4, to arrive at the stated result. □

The corresponding example of the saddle point equation for the isotropic XY model is

$$\epsilon = \frac{1}{\pi} \int_0^{\pi/2} dq \, \cos q \tanh(\xi \cos q) \ , \tag{46}$$

and that for the Ising model in a transverse field is

$$\epsilon = \frac{1}{\pi} \int_0^{\pi} dq \, \epsilon_q \frac{\frac{x+\cos q}{\epsilon_q} + \tanh(2\xi\epsilon_q)}{1 + \frac{x+\cos q}{\epsilon_q} \tanh(2\xi\epsilon_q)} \ . \tag{47}$$

The first of the more obvious properties concerns the convexity of the measure arising in the thermodynamic limit,

Theorem 5 *The leading order of the negative logarithm of the weight function $u(\epsilon)$ is convex for all real energies ϵ.*

This follows from the relationship of $u(\epsilon)$ to the stationary point

$$\frac{d}{d\epsilon} u(\epsilon) = N\xi(\epsilon) \ , \tag{48}$$

and the definition

$$\epsilon = F'(\xi) \ . \tag{49}$$

Now it can be easily seen that $F''(t) > 0$ for t real and the Hermitian Hamiltonian using the definition of $F(t)$ in terms of the expectation value $NF(t) = \ln\langle \exp(tH) \rangle$.□

Some detailed, yet general information, concerning the extensive measure in the neighbourhood of the ground state is available. This arises from consideration of the overlap of the trial state with the true ground state[31], and its relation to the Horn-Weinstein function $E(t) \equiv F'(-t)$ via

$$|\langle \Psi_{GS} | \psi_0 \rangle|^2 = \exp\left\{ -N \int_0^{\infty} dt \, [E(t) - E(\infty)] \right\} \ . \tag{50}$$

In general the limit $E(t)$ as $t \to \infty$ will exist, and is the ground state energy, and so the asymptotic properties of $E(t)$ for $\Re(t) > 0$ as this tends to infinity is a means of classifying systems. This equivalent to the asymptotic properties of $\epsilon(\xi) - \epsilon(-\infty)$ as $\xi \to -\infty$ (we denote the Ground State Energy by ϵ_0, which is also the same as $\epsilon(-\infty)$). In general the overlap is non-zero, so that $E(t) - E(\infty) \in L^1[0, \infty)$ but it is possible at isolated points that this is not true (critical points in the model for example) and the overlap may vanish. For example the overlap squared in the case of the isotropic XY model is $2^{-N/2}$ and that for the Ising model in a transverse field is

$$\exp\left\{ \frac{N}{2\pi} \int_0^{\pi} dq \, \ln\left(\frac{\epsilon_q + x + \cos q}{2\epsilon_q} \right) \right\} \ . \tag{51}$$

Where the overlap is non-zero then several possibilities for the asymptotic behaviour exist, which do actually arise in the exact solutions of the example models -

- gapless case, isotropic XY and critical Ising Model in a transverse Field, Ref.[32, 23]: At a critical point, the first excited state gap vanishes and

$$\epsilon - \epsilon_0 \sim A|\xi|^{-\gamma} \ , \tag{52}$$

as $\xi \to -\infty$ and if the overlap is finite then $\Re(\gamma) > 1$. Therefore the weight function at the bottom of the spectrum takes the following form

$$w(\epsilon) \sim (\epsilon - \epsilon_0)^{-\frac{1+\gamma}{2\gamma}} \exp\left\{ N \frac{b}{1-1/\gamma} (\epsilon - \epsilon_0)^{1-1/\gamma} \right\} \ , \tag{53}$$

This measure is integrable on $(\epsilon_0, \epsilon_\infty)$ because of the above condition $\Re(\gamma) > 1$ and has a branch point at the ground state energy ϵ_0.

- gapped case 1, Ising Model in a transverse Field, in the ordered phase with the disordered trial state, Ref.[23]:
if the gap is finite then one possibility is that

$$\epsilon - \epsilon_0 \sim A e^{-\Delta|\xi|} \ , \tag{54}$$

as $\xi \to -\infty$ and where the excited state gap $\Delta > 0$. One can show that the weight function near the bottom edge of the spectrum is analytic having the form

$$w(\epsilon) \sim \frac{1}{\Gamma(N \frac{[\epsilon - \epsilon_0]}{\Delta} + 1)} \ . \tag{55}$$

- gapped case 2, Ising Model in a transverse Field, in the disordered phase with the disordered trial state, Ref.[23]:
and yet another type of gap behaviour exists

$$\epsilon - \epsilon_0 \sim A|\xi|^{-\gamma} e^{-\Delta|\xi|} \ , \tag{56}$$

The leading order behaviour of the weight function in this case is

$$w(\epsilon) \sim (\epsilon - \epsilon_0)^{-1/2 - N(\epsilon - \epsilon_0)} \left[-\log(\epsilon - \epsilon_0) \right]^{-N\gamma(\epsilon - \epsilon_0)} \ , \tag{57}$$

which again has a branch point at the bottom edge of the spectrum.

So generally we find the support of the measure is bounded which excludes a number of weight function types such as the Freud or Erdös weights, but that the weight functions belong to the Szegö class on $[\epsilon_0, \epsilon_\infty]$,

$$\int_{\epsilon_0}^{\epsilon_\infty} d\epsilon \, \frac{\log w(\epsilon)}{\sqrt{[\epsilon_\infty - \epsilon][\epsilon - \epsilon_0]}} > -\infty \ . \tag{58}$$

V. Exactly Solvable Lanczos Process

In this section we derive how the exact Lanczos functions $\alpha(s)$ and $\beta^2(s)$ can be constructed directly from the knowledge of the connected Moments or Cumulants, or more specifically from the Cumulant Generating Function. This is the initial data that one uses in any analysis of quantum Many-Body Systems with this approach, and for soluble models the full Generating Function may be available. However if this is not the case then one would use a set of low order Cumulants, up to a given order.

As a first step we recast the Hankel determinants into Selberg Integral form, from the classical result[9]

$$\Delta_n(t) = \frac{1}{(n+1)!}\int_{-\infty}^{+\infty} \prod_{k=1}^{n+1} d\rho(\epsilon_k)\, e^{Nt\sum_{k=1}^{n+1}\epsilon_k} \prod_{1\le i<j\le n+1} |\epsilon_i - \epsilon_j|^2 \ . \tag{59}$$

For the steps leading to the two conditions which will define the Lanczos functions we follow Chen and Ismail[13]. A similar approach, but just confined to the evaluation the Hankel determinants, was taken in References [33, 34]. The Hankel determinant can be recast into the form of a partition function, which is,

$$\Delta_n(t) = \frac{1}{(n+1)!}\int_{-\infty}^{+\infty} \prod_{i}^{n+1} d\epsilon_i\ \exp\left\{ -\sum_{i}^{n+1} u(\epsilon_i) + Nt\sum_{i}^{n+1}\epsilon_i + 2\sum_{i<j}^{n+1}\ln|\epsilon_i-\epsilon_j| \right\} \ . \tag{60}$$

One should observe that both $\sum_i^{n+1} u(\epsilon_i)$ and $Nt\sum_i^{n+1}\epsilon_i$ are of order $(n+1)N$ whilst the remaining term in the argument $\sum_{i<j}^{n+1}\ln|\epsilon_i-\epsilon_j|$ is of order $(n+1)^2$, so that the only relative scaling that remains nontrivial is one in which n/N is fixed. The alternatives would lead to completely trivial consequences. The leading order term for this Hankel determinant as $n, N\to\infty$ is given by a steepest descent approximation (see Ref. [30] section IX.5)

$$\Delta_n(t) = \frac{(2\pi)^{n+1}}{(n+1)!}\left|\frac{\partial^2 f}{\partial\epsilon_i^0\partial\epsilon_j^0}\right|^{-1/2} e^{-f(\epsilon^0)}\left[1+\mathrm{O}(1/n,1/N)\right] \ , \tag{61}$$

where the function $f(\epsilon)$ is defined as

$$f(\epsilon) = \sum_{i}^{n+1} u(\epsilon_i) - Nt\sum_{i}^{n+1}\epsilon_i - 2\sum_{i<j}^{n+1}\ln|\epsilon_i-\epsilon_j| \ , \tag{62}$$

and the saddle points $\{\epsilon_i^0\}_{i=1}^{n+1}$ are given by

$$u'(\epsilon_i^0) = Nt + 2\sum_{i\neq j}^{n+1}\frac{1}{\epsilon_i^0-\epsilon_j^0} \ . \tag{63}$$

One can easily show that the Hessian in Eq. (61) is positive definite given that $u(\epsilon)$ is convex. One can carry the continuum limit further by describing the saddle points as a charged fluid whose dynamics are governed by an Energy Functional $F[\sigma]$

$$\exp\left(-f(\epsilon^0)\right) \xrightarrow[n,N\to\infty]{} \exp\left(-F[\sigma_0]\right) \ , \tag{64}$$

with a charge density $\sigma(\epsilon)$ defined on an interval of integration which is to be determined, $I=(\epsilon_-,\epsilon_+)$. The energy functional takes the following form

$$F[\sigma] = \int_I d\epsilon\sigma(\epsilon)\left[u(\epsilon)-Nt\epsilon\right] - \int_I d\epsilon\int_I d\epsilon'\sigma(\epsilon)\ln|\epsilon-\epsilon'|\sigma(\epsilon') \ , \tag{65}$$

where the single particle confining potential is controlled by the OPS measure and the two-body interaction is a logarithmic type. The result of minimising this Functional yields the following singular integral equation for the Charge Density

$$u'(\epsilon) - Nt = 2\,\mathrm{PV}\int_I d\epsilon' \frac{\sigma_0(\epsilon')}{\epsilon-\epsilon'}\ . \tag{66}$$

The solution of this integral equation for the Minimal Charge Density $\sigma_0(\epsilon)$ can be found exactly and is

$$\sigma_0(\epsilon) = \frac{\sqrt{(\epsilon_+-\epsilon)(\epsilon-\epsilon_-)}}{2\pi^2}\,\mathrm{PV}\int_I d\epsilon' \frac{u'(\epsilon')-Nt}{(\epsilon'-\epsilon)\sqrt{(\epsilon_+-\epsilon')(\epsilon'-\epsilon_-)}}\ . \tag{67}$$

There are two conditions arising from this solution -

- the first is a Supplementary Condition which is necessary for the charge density solution to be well defined throughout the interval I

$$0 = \int_I d\epsilon \frac{u'(\epsilon)-Nt}{\sqrt{(\epsilon_+-\epsilon)(\epsilon-\epsilon_-)}}\ , \tag{68}$$

- and the Normalisation Condition which simply counts the number of Lanczos steps

$$n = \frac{1}{2\pi}\int_I d\epsilon\ \epsilon \frac{u'(\epsilon)-Nt}{\sqrt{(\epsilon_+-\epsilon)(\epsilon-\epsilon_-)}}\ . \tag{69}$$

Using this solution for the charge density one can substitute this into the original defining equations for the Hankel determinants (the leading order approximations) and establish that the Lanczos functions are simply defined by the interval I in this way, $\epsilon_\pm = \alpha \pm 2\beta$.

Theorem 6 *The Lanczos functions are given implicitly by the two integral equations*

$$0 = \int_{\alpha-2\beta}^{\alpha+2\beta} d\epsilon \frac{\xi(\epsilon)}{\sqrt{4\beta^2-(\epsilon-\alpha)^2}}\ , \tag{70}$$

$$s = \frac{1}{2\pi}\int_{\alpha-2\beta}^{\alpha+2\beta} d\epsilon \frac{\epsilon\xi(\epsilon)}{\sqrt{4\beta^2-(\epsilon-\alpha)^2}}\ , \tag{71}$$

where the model dependent equation for the stationary point $\xi(\epsilon)$ is given by Eq. (49).

This theorem follows from the previous conditions, namely Eqs. (68,69), and the result for the logarithmic derivative of the weight function,

$$u'(\epsilon) = N\xi(\epsilon) + \mathrm{O}(\log N)\ . \tag{72}$$

□

Usually this later equation for the saddle point is also an implicit equation and invariably a nonlinear one. In our derivation the scaling $s = n/N$ remains finite whilst $n, N \to \infty$ emerges naturally and in fact it is difficult to see how one could avoid this confluence.

We now give an alternative result for the Lanczos functions which is based on the time evolution of the Lanczos L-function.

Theorem 7 *The Lanczos L-function, in the thermodynamic limit is the solution of the following integro-differential equation*

$$L(s,t) = \int_0^s dr\, r D_t^2 \log L(s-r,t) + sF^{(2)}(t) \ , \tag{73}$$

and the two Lanczos functions are derivable from this via

$$\begin{aligned} \alpha(s) &= \int_0^s dr\ D_t \log L(r,0) + F'(0) \ , \\ \beta^2(s) &= L(s,0) \ . \end{aligned} \tag{74}$$

The integro-differential equation is simply derived from the discrete recurrence, namely Eq. (24), after making the observation that the $j = n$ term involving $L_0(t)$ has to be separated from the sum because it encompasses the initial conditions and is itself not generated by the recurrence.□

Finally we give a result equivalent to the theorem above, but which involves only scaled forms of the Hankel determinants $\Delta_n(N,t)$ and is the differential analogue of the above Theorem.

Definition 4 *We make the following definition for $\delta(n,N,t)$ in terms of the Hankel Determinant,*

$$\Delta_n(N,t) = N^{n(n+1)} \left[\delta(n,N,t)\right]^{N^2} \ , \tag{75}$$

for $n \geq 1$ and $\Delta_0(t) = [\delta(0,t)]^N$.

Lemma 3 *The function $\delta(n,N,t)$ is well defined in the scaling limit $n, N \to \infty$.*

This follows naturally from the relation of the $\Delta_n(t)$ and the Lanczos L-function as given in Eq. (22), and the well defined scaling of this latter function as demonstrated in the Theorem 3 above. □

Then we have the following result -

Theorem 8 *The Lanczos $\delta(s,t)$-function satisfies the following partial differential equation in the thermodynamic limit*

$$\exp\left\{D_s^2 \log \delta(s,t)\right\} = D_t^2 \log \delta(s,t) \ , \tag{76}$$

with the boundary condition

$$\lim_{s \to 0^+} \frac{\log \delta(s,t)}{s} = F(t) \qquad \forall\, t \in \mathbb{R}^+ \ , \tag{77}$$

The Lanczos functions are given by

$$\begin{aligned} \alpha(s) &= D_t D_s \log \delta(s,t)|_{t=0} \ , \\ \beta^2(s) &= \exp\left\{D_s^2 \log \delta(s,0)\right\} \ . \end{aligned} \tag{78}$$

Using the scaling relation above, Eq. (75), and the equation of motion for $\Delta_n(t)$, Eq. (27), the result follows. □

These last two theorems relate to the dynamics of a nonlinear continuum Toda Lattice in one space domain $s \in \mathbb{R}^+$ and one time domain t, with boundary conditions defined at the origin $s = 0$ for all times t by the cumulant generating function $F(t)$. The object is then to find the Lanczos functions $\alpha(s), \beta^2(s)$ from a solution of this system, wherein these functions are directly related to the solution at a given time $t = 0$ over all spatial points $s > 0$.

VI. The Taylor Series Expansion

The investigation of the Taylor series expansion of the Lanczos coefficients about $s = 0$, is an essential element in the application of this Lanczos method, as was indicated earlier, where one has only a finite set of low order cumulants available, say for non-integrable models. Therefore in this case one can only construct a truncated Taylor series expansion and so issues concerning convergence, the radius of convergence of the series, and whether one can extrapolate immediately arise. In addition one would like a direct algorithm relating the cumulants to the Lanczos functions from a purely practical point of view.

We define the Taylor series expansion of the two Lanczos functions by two new sequences of coefficients,

$$
\begin{aligned}
\alpha(s) &= c_1 + \sum_{n=0}^{\infty} a_n s^{n+1} \ , \\
\beta^2(s) &= \sum_{n=0}^{\infty} b_n s^{n+1} \ .
\end{aligned}
\tag{79}
$$

In order to find these coefficients one could use either of the two general solutions for the Lanczos process, Eqs. (70,71) or Eq. (73), and the two methods are presented below.

The first step involves the inversion of the following Taylor series expansion

$$
\epsilon = c_1 + \sum_{n=1} \frac{c_{n+1}}{n!} \xi^n \ , \tag{80}
$$

for $\xi(\epsilon)$, namely the coefficients e_k appearing in

$$
\xi = \sum_{k=1} e_k (\epsilon - c_1)^k \ . \tag{81}
$$

The coefficients c_n appearing in Eq. 80 are the cumulant coefficients. The existence of this inverse function is guaranteed because the second cumulant $c_2 > 0$ in all systems and we assume that the saddle point function, Eq. (49), is analytic in the neighbourhood of $\xi = 0$. The next step involves the solution of the two recurrences

$$
\begin{aligned}
0 &= \sum_{k=1} e_k \sum_{m=0}^{\lfloor k/2 \rfloor} \binom{k}{2m} \frac{(1/2)_m}{m!} (\alpha - c_1)^{k-2m} (4\beta^2)^m \ , \\
2s &= \sum_{k=1} e_k \sum_{m=0}^{\lfloor (k-1)/2 \rfloor} \binom{k}{2m+1} \frac{(1/2)_{m+1}}{(m+1)!} (\alpha - c_1)^{k-2m-1} (4\beta^2)^{m+1} \ ,
\end{aligned}
\tag{82}
$$

which are used to solve for the coefficients a_n, b_n appearing in Eq. (79).

In the second method we define a continuum version of the coefficients that are defined in Eq. (33) in the following way

$$
\log \frac{L(s,t)}{s l_1(t)} = \log \left(1 + \sum_{p \geq 1} \frac{l_{p+1}}{l_1} s^p \right) \equiv \sum_{p \geq 1} m_p(t) s^p \ , \tag{83}
$$

and the inverse of Eq. (34) in an explicit form

$$
\frac{l_{p+1}}{l_1} = \sum_{\sum_i q_i r_i = p} \prod_i \frac{1}{q_i!} m_{r_i}^{q_i} \ . \tag{84}
$$

From these relations one can find a hierarchy of equations for these coefficients

$$
\begin{aligned}
l_1(t) &= F''(t) \ , \\
l_2(t) &= \frac{F^{(2)}F^{(4)} - (F^{(3)})^2}{2(F^{(2)})^2} \ , \\
l_{p+2}(t) &= \frac{m''_p(t)}{(p+2)(p+1)} = l_1(t) \sum_{\sum_i q_i r_i = p+1} \prod_i \frac{m_{r_i}^{q_i}}{q_i!} \qquad \text{for } p \geq 1 \ .
\end{aligned}
\tag{85}
$$

Thus one can verify from the solution for the initial value problem above that the general Taylor series coefficients are given by

$$
\begin{aligned}
[(n+1)!]^2 c_2^{3n+1} a_n &= \sum_{\lambda \vdash 2n+1} A(n;\lambda) \prod_{i=0}^{2n+1} c_{2+i}^{a_i} \\
(n+1)!n!c_2^{3n-1} b_n &= \sum_{\lambda \vdash 2n} B(n;\lambda) \prod_{i=0}^{2n} c_{2+i}^{a_i} \ ,
\end{aligned}
\tag{86}
$$

where the coefficients labeled by the partition $\lambda = (1^{a_1}.2^{a_2} \ldots i^{a_i})$, denoted by $A(n;\lambda), B(n;\lambda)$, are listed in Table(1) of the Appendix. There are constraints operating in the above equations, namely $\sum_{i=1}^{2n+1} i a_i = \sum_{i=0}^{2n+1} a_i = 2n+1$ for the first relation and $\sum_{i=1}^{2n} i a_i = \sum_{i=0}^{2n} a_i = 2n$ for the second.

Clearly the Taylor series expansion of the Lanczos functions has low order coefficients which are constructed from the low order cumulants, and is a form of a linked cluster expansion. However it is not just a simple linked cluster expansion as in the Taylor series expansion of the Cumulant Generating Function, but involves a subtle interplay and cancellation of all cumulants below a given order.

VII. General Properties

There are some very general properties that the Lanczos process in the thermodynamic limit and the associated Lanczos functions satisfy and we examine these now. Some are quite obvious and not particularly surprising, however we state these for completeness sake, while there are some other properties which are not so immediate but very important nevertheless.

The next, and natural, property concerns the monotonicity of the two envelope functions $\epsilon_{\pm}(s) = \alpha(s) \pm 2\beta(s)$.

Theorem 9 *The envelope functions $\epsilon_{+}(s), \epsilon_{-}(s)$ are monotonically increasing and decreasing functions of real, positive s respectively.*

This follows from a recasting of the normalisation condition in the following way

$$2\pi s = \int_{\xi_-}^{\xi+} d\xi \sqrt{[\epsilon(\xi_+) - \epsilon(\xi)][\epsilon(\xi) - \epsilon(\xi_-)]} \ , \tag{87}$$

where the $\xi_{\pm}$ are defined by $\epsilon(\xi_{\pm}) = \epsilon_{\pm}$. Now it is straight forward to write the explicit forms for the derivatives of the envelope functions with respect to s as

$$\begin{aligned} \frac{d\epsilon_+}{ds} &= 4\pi \Big/ \int_{\xi_-}^{\xi_+} d\xi \sqrt{\frac{\epsilon(\xi) - \epsilon(\xi_-)}{\epsilon(\xi_+) - \epsilon(\xi)}} \ , \\ \frac{d\epsilon_-}{ds} &= -4\pi \Big/ \int_{\xi_-}^{\xi_+} d\xi \sqrt{\frac{\epsilon(\xi_+) - \epsilon(\xi)}{\epsilon(\xi) - \epsilon(\xi_-)}} \ , \end{aligned} \tag{88}$$

so that the stated properties are evident.□

It is clear that the envelope functions $e_{\pm}(s)$ are bounded in the following ways, $\epsilon_-(s) \geq \epsilon_0$ and $\epsilon_+(s) \leq \epsilon_\infty$.

The 3-term recurrence which serves as one of the definitions of the Orthogonal Polynomials themselves is now going to take a definite limiting form when $n, N \to \infty$ such that s is finite. This is going to lead to a scaling form for one set of the Polynomials themselves, which would be more correctly termed orthogonal functions $p(s,\epsilon)$. Heuristically one can see how this arises by the following argument. If one ensures that Lanczos densities are employed and the following scaling of the polynomials thus $P_n(E) = N^n p_n(\epsilon)$, then the 3-term recurrence becomes

$$p_{n+1}(\epsilon)/p_n(\epsilon) + \beta_n^2 \frac{1}{p_n(\epsilon)/p_{n-1}(\epsilon)} = \epsilon - \alpha_n \ . \tag{89}$$

Now these ratios are approximated by

$$\frac{p_{n+1}(\epsilon)}{p_n(\epsilon)} \sim \exp\left(\frac{1}{N} \frac{\partial}{\partial s} \ln p(s,\epsilon) \right) \ , \tag{90}$$

for arguments $\epsilon \in \mathbb{C} \backslash \mathrm{Supp}[d\rho]$. So that in the asymptotic regime the recurrence becomes

$$\exp\left(\frac{1}{N} \frac{\partial}{\partial s} \ln p(s,\epsilon) \right) + \beta^2(s) \exp\left(-\frac{1}{N} \frac{\partial}{\partial s} \ln p(s,\epsilon) \right) \sim \epsilon - \alpha(s) \ , \tag{91}$$

whose solutions are

$$p^{\pm}(s,\epsilon) \sim p(0) \exp\left\{ N \int^s dt \ln \frac{1}{2} \left[\epsilon - \alpha(t) \pm \sqrt{(\epsilon - \alpha(t))^2 - 4\beta^2(t)} \right] \right\} \ . \tag{92}$$

These are the corresponding results for the ratio $P_n(x)/P_{n+1}(x)$ or n-th root $\sqrt[n]{P_n(x)}$ asymptotics of generic Orthogonal Polynomials as $n \to \infty$[9, 11, 35, 36, 37], or the scaled Orthogonal Polynomials[14], but are rather different due to the particular nature of Many-Body Orthogonal Polynomials.

Theorem 10 *Given the scaling behaviour of the Lanczos coefficients, and that they are bounded for $n, N \to \infty$, then the n-th root of the denominator Orthogonal Polynomials $p_n(\epsilon)$ have the limiting form uniformly for ϵ in compact subsets of $\mathbb{C}\backslash\mathrm{Supp}[d\rho]$.*

$$p(s,\epsilon) \equiv \lim_{n,N\to\infty} |p_n(N,\epsilon)|^{1/N} = \exp\left\{ \int_0^s dt \;\ln\frac{1}{2}\left[\epsilon-\alpha(t) + \sqrt{(\epsilon-\alpha(t))^2-4\beta^2(t)}\right] \right\} \tag{93}$$

The proof of this parallels the one constructed by van Assche in Ref. [14] through the use of Turán Determinants,

$$D_n \equiv p_n^2 - p_{n+1}p_{n-1} \tag{94}$$

One can show that these obey the following recurrence relation

$$D_n = \beta_n^2 D_{n-1} + (\alpha_n - \alpha_{n-1})p_n p_{n-1} + (\beta_n^2 - \beta_{n-1}^2)p_n p_{n-2} \tag{95}$$

Using the partial fraction decomposition of the ratio of two successive Orthogonal Polynomials one can also find a bound on this ratio

$$\left|\frac{p_{n-1}(\epsilon)}{p_n(\epsilon)}\right| \le \frac{C}{d} \qquad \forall\, n \tag{96}$$

for all $\epsilon \in K$ where the compact set $K \subset \mathbb{C}\backslash\mathrm{Supp}[d\rho]$ and d is the distance between this set and the interval $[\epsilon_0, \epsilon_\infty]$, and C is a positive constant. Using Eq. (95) we have

$$\left|\frac{D_n}{p_n^2}\right| \le \sup_n(\beta_n^2)\frac{C^2}{d^2}\left|\frac{D_{n-1}}{p_{n-1}^2}\right| + |\alpha_n - \alpha_{n-1}|\frac{C}{d} + |\beta_n^2 - \beta_{n-1}^2|\frac{C^2}{d^2} \tag{97}$$

Given the scaling form of the Lanczos coefficients the ratio $|D_n/p_n^2| \to 0$ as $n, N \to \infty$ uniformly in ϵ whenever d is large enough. This means that $|p_{n-1}/p_n|$ and $|p_n/p_{n+1}|$ tend to the same accumulation point which we denote by $p(s,\epsilon)$. This point is given by the solution of the quadratic equation $p + \beta^2(s)/p = \epsilon - \alpha(s)$, and the positive branch of the solution must be taken as $p \to \infty$ when $\epsilon \to \infty$. The functions $p(s,\epsilon)$ are analytic functions of $\epsilon \in K$ which are uniformly bounded, so the restriction on d can be lifted to being only non-zero. The behaviour of the n-th ratio then gives the n-th root behaviour directly as

$$|p_n|^{1/N} = \exp\left\{ \frac{1}{N}\sum_{k=1}^{n} \log\left|\frac{p_k(\epsilon)}{p_{k-1}(\epsilon)}\right| \right\} \tag{98}$$

The asymptotic behaviour that we have found applies to the denominator OP only as can be seen from the observation that $p_1 = \epsilon - c_1$ and $p_2 = (\epsilon - c_1)^2 - c_3/c_2 N(\epsilon - c_1) - c_2/N$, while

$$\left[\epsilon-\alpha(s) + \sqrt{(\epsilon-\alpha(s))^2-4\beta^2(s)}\right] \xrightarrow[s\to 0]{} \frac{1}{\epsilon - c_1}\left((\epsilon-c_1)^2 - c_3/c_2 N(\epsilon - c_1) - c_2/N\right) \;. \tag{99}$$

This establishes the result.□

VIII. Summary

In this work we have demonstrated the general scaling behaviour of the Lanczos Process as applied to Many-Body Systems when the process is taken to convergence and the thermodynamic limit taken. We also find explicit constructions of the limiting Lanczos coefficients in two equivalent formulations, from an initial exact solution of the moment problem, that is to say the cumulant generating function for the system. There are explicit examples where the CGF can be found and the whole Lanczos process explicitly realised. Furthermore we have given the corresponding results for the associated Orthogonal Polynomial system and the measure in this regime, quite generally. However we must emphasise that these results apply only to the bulk properties, that is to say the ground state properties that scale extensively and the spectral properties in the interior (the "bulk") of the spectrum. So this does not include the delicate scaling behaviour at the edges of the spectrum, nor in the neighbourhood of singularities - this theory would have to be extended to treat the excited state gaps near the bottom of the spectrum. A number of general theorems are given which constrain the behaviour of the Lanczos functions, and the process in general. We also indicate how a number of such constraints operating can lead to some concrete realisations or scenarios that the Lanczos process can present, namely its behaviour at a critical point in the model under study. This is a significant step on the way to the goal of a rigorous classification of Many-Body Systems in terms of their character via the Lanczos process. Other important questions that arise in the treatment of non-integrable models, for which the general results presented here have suggested some answers, are the questions of the choice of trial state, the rate of convergence of the truncated Lanczos process and how one might accelerate its convergence given some independent qualitative knowledge.

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Acknowledgements

One of the authors (NSW) would like to acknowledge the support of a Australian Research Council large Grant whilst this work was performed, and the hospitality of Service de Physique Théorique, Centre d'Etudes Nucléaires de Saclay.

Appendix

We list here the coefficients of the Taylor series expansion for the Lanczos Coefficients, labelled by the partitions of integers, according to the definition of Eq.(86).

1	a_0	$\lambda =$	$A(0;\lambda) =$
		1	1
2	b_1	$\lambda =$	$B(1;\lambda) =$
		2	1
		1^2	-1
3	a_1	$\lambda =$	$A(1;\lambda) =$
		1^3	3
		2.1	-4
		3	1
4	b_2	$\lambda =$	$B(2;\lambda) =$
		1^4	-12
		2.1^2	21
		2^2	-4
		3.1	-6
		4	1
5	a_2	$\lambda =$	$A(2;\lambda) =$
		1^5	81
		2.1^3	-174
		3.1^2	48
		$2^2.1$	70
		4.1	-9
		3.2	-17
		5	1
6	b_3	$\lambda =$	$B(3;\lambda) =$
		1^6	-567
		2.1^4	1449
		3.1^3	-414
		$2^2.1^2$	-872
		4.1^2	84
		$3.2.1$	304
		5.1	-12
		2^3	70
		4.2	-26
		3^2	-17
		6	1

7	a_3	$\lambda =$	$A(3;\lambda) =$
		1^7	5805
		2.1^5	-17190
		3.1^4	4815
		$2^2.1^3$	13940
		4.1^3	-990
		5.1^2	150
		$3.2.1^2$	-5470
		$2^3.1$	-2680
		$3^2.1$	425
		$4.2.1$	680
		6.1	-16
		3.2^2	640
		5.2	-44
		4.3	-66
		7	1
8	b_4	$\lambda =$	$B(4;\lambda) =$
		1^8	-58050
		2.1^6	195345
		3.1^5	-55710
		$2^2.1^4$	-197470
		$3.2.1^3$	85430
		4.1^4	11745
		5.1^3	-1890
		$2^3.1^2$	60580
		$3^2.1^2$	-8020
		$4.2.1^2$	-12520
		6.1^2	230
		$3.2^2.1$	-22820
		$4.3.1$	1860
		$5.2.1$	1200
		7.1	-20
		2^4	-2680
		4.2^2	1320
		$3^2.2$	1705
		6.2	-60
		5.3	-110
		4^2	-66
		8	1

Table 1: The coefficients in the Taylor series expansion for the Lanczos functions $\alpha(s)$ and $\beta^2(s)$, as defined in Eq.(86), and the labels denoting the partitions λ of the positive integers.